1,2,3,5-Tetrachlorobenzene 634-90-2 | DTXSID1026089

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%	Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 3.25e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.77e-01

Confidence level: 6.27e-01

Nearest Neighbors from the Training Set

Image not found

Docosane

Measured: 5.53e-02 Predicted: 4.97e-06

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1,2,4,5-Tetramethylbenzene

Measured: 5.40e-03 Predicted: 1.01

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Silane, tetraethyl-Measured: 3.90e-02 Predicted: 7.80

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Phthalide

Measured: 2.10e-01 Predicted: 2.25e-03

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Isoquinoline

Measured: 4.60e-01 Predicted: 2.62e-02